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NASA TM X-52944

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PROJECTED HARTREE-FOCK SPECTRA WITH WOOD-SAXON BASIS FUNCTIONS

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TECHNICAL PAPER proposed for presentation at
Winter Meeting of the American Physical Society
Stanford, California, December 28-31, 1970

E-6098

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ABSTRACT

We have previously reported the results of an investigation of intrinsic Hartree-Fock spectra and projected nuclear properties, such as E2 rates and inelastic scattering cross sections, when basis functions with Wood-Saxon radial dependence are used. It was found that predicted values of properties sensitive to the long range behavior of the wave functions were improved by the use of a Wood-Saxon basis. Since the basis functions are normalized to unity, the short-range behavior of the wave function, and hence the energies, should be affected. This point is investigated by comparison of projected Hartree-Fock spectra using basis functions having harmonic oscillator and Wood-Saxon radial dependence.

INTRODUCTION

The study of nuclear properties based on the Hartree-Fock method has been limited almost entirely to calculations made with harmonic oscillator (HO) model spaces. This is true in spite of the well-known incorrect asymptotic behavior of the basis states. Recently, the present authors investigated the use of Wood-Saxon (WS) basis functions in Hartree-Fock studies.[1] It was found that the use of Wood-Saxon functions yielded improved results for some observables relative to those obtained with HO functions.[1,2] Those calculations were made with an inert ^{16}O core, and only the 2s-ld shell model states were used as the basis space. It has been found, however, that core polarization effects make important contributions to many nuclear properties when HO functions are used and thus such effects should be investigated for the WS case also. In the earlier work the Wood-Saxon results were compared with similar ones obtained using HO functions. The choice of oscillator parameter posed something of a problem but at length two physically meaningful parameters were chosen. One of the parameters (b = 1.69 fm) yields peaks and nodes which match those of the Wood-Saxon functions; this is probably the most logical choice for purposes of comparison. The other (b = 1.924 fm) was chosen to reproduce approximately binding energies, gaps, and intrinsic single particle energies obtained in the WS results.

Since the WS functions do not fall off as rapidly as the HO functions, one would expect to find an improvement in the nuclear properties which are sensitive to the long range behavior of the nuclear wave function. This was found to be the case for the study using an inert core.[2] However, the long range behavior should also manifest itself in properties such as energies which are sensitive to the short range behavior of the wave function. This is due to the fact that the single particle basis functions are normalized to unity.

In this article we compare the results of HF calculations made with the three model spaces defined above. The assumption of an ^{16}O core is dropped, making it possible to study the effects of core polarization. Several projected properties such as RMS radius, E2 rates, and projected energy spectra are examined and compared for the three spaces in an effort to determine any effect which long range properties may induce in the energy spectra.

Calculation

The HF model space used in the calculations consisted of the shell model states: $1s_{1/2}$, $1p_{1/2}$, $1p_{3/2}$, $2s_{1/2}$, $1d_{5/2}$, and $1d_{3/2}$. The evaluation of the 2-body matrix elements for the harmonic oscillator functions is straightforward; however, when WS functions are used, their evaluation requires special techniques which have been discussed in an earlier publication. The nucleon-nucleon interaction used in these calculations is the Volkov force[3]

$$V(|\vec{r}_1 - \vec{r}_2|) = \left\{\alpha + \beta\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \gamma\vec{\tau}_1 \cdot \vec{\tau}_2 + \delta\vec{\sigma}_1 \cdot \vec{\sigma}_2\vec{\tau}_1 \cdot \vec{\tau}_2\right\} f(|\vec{r}_1 - \vec{r}_2|)$$

where

$$f(|\vec{r}_1 - \vec{r}_2|) = -78\ e^{-(|\vec{r}_1-\vec{r}_2|^2/2.25)} + 82.5\ e^{-(|\vec{r}_1-\vec{r}_2|^2/0.64)}$$

This force (with $\alpha = 0.1875$, $\beta = 0.0775$, $\gamma = 0.2025$, $\delta = 0.1775$) has been found to yield good saturation properties for the p-shell nuclei.

Most of the nuclear properties which we shall be concerned with involve the evaluation of reduced matrix elements (between projected HF states, $\psi_{JM} = P^J_{MK}\Phi_K$) of sums of single-particle operators which may be expanded in terms of spin-angle tensors with coefficients $\omega_{LSJ}(r)$. Reduced matrix elements of such an operator may be expressed as[4]

$$\left\langle J_f \middle\| \sum_{n=1} \Omega(n) \middle\| J_i \right\rangle = \sum_{LS} \int_0^\infty \rho^{if}_{LSJ}(r)\omega_{LSJ}(r)r^2\, dr$$

where the structure information is contained in the transition densities $\rho^{if}_{LSJ}(r)$. Of course the calculation of the projected energy spectrum also involves two-body operators, and is therefore more complicated. One must calculate

$$E_J = \left\langle \varphi_k \middle| HP^J_{KK} \middle| \varphi_K \right\rangle \Big/ \left\langle \varphi_K \middle| P^J_{KK} \middle| \varphi_K \right\rangle$$

where the Hamiltonian, H, is the sum of one-body (kinetic energy) and two-body (potential) operators. The calculation of this quantity is discussed in detail elsewhere.[5]

RESULTS AND DISCUSSION

The radial functions for some of the single-particle states are compared in Figures 1-3. As noted earlier the WS functions are generally depressed (relative to the HO) at small values of r, but fall off less rapidly at larger values. This is a consequence of normalization to unity.

The intrinsic and projected quantites for ^{20}Ne, ^{24}Mg, ^{28}Si, and ^{32}S are presented in Tables I and II. First of all we note that in all cases the HO results yield a lower HF energy (more binding) than the WS. This is due to the fact that the short range part of the WS function is depressed relative to that of the HO type. In Table I, we note a significant difference in the intrinsic properties (E_{HF} and Δ), as was found for the inert core study. A similar difference is noted for the projected properties, but comparison with Table III reveals that the WS results are in better agreement with experiment. In Table II (b = 1.924 fm.) the intrinsic and projected properties are seen to be in much closer agreement than in the previous case. However, the radii are generally too large for this oscillator parameter.

The projected spectra for the nuclei of interest are presented in Figures 4-7. In all cases, the spectra for the two oscillator parameters differ very little; furthermore, the Wood-Saxon spectra are only slightly different from the HO results. Comparison with experiment reveals that the predicted spectra in all cases are too compressed. This is not surprising, however, due to the small size of the model space.

The ^{20}Ne Wood-Saxon result show a somewhat peculiar distribution of the different amounts of the various J-components in the intrinsic state. This gives rise to an unusual spectrum, which does not appear to be rotational. The wave function for this state was examined very closely for errors and appears to be correct. It may be that the particular solution obtained is not the best HF self-consistent solution which can be found, but represents only a local minimum of the HF energy surface.

CONCLUDING REMARKS

The purpose of this work has been to determine whether the use of WS basis functions in HF calculations would affect the projected energy spectra. Previous studies have established that the long range behavior of these functions modified the single particle spectra slightly and lowers the HF energy relative to HO results. Our present findings show that absolute values of the energy spectra are higher for the WS functions but that the relative separations of the projected energy levels are not affected significantly.

However, this study has provided an additional valuable result, namely that one need not necessarily examine such hard-to-calculate properties as projected energies in order to test the relative validity of the various aspects of a nuclear model. Due to the small number of basis states in the model space it was not expected that the projected spectra would agree very well with experiment. However, it was rather surprising to find that the large differences in intrinsic states and single particle properties did not manifest themselves significantly in the energy spectra. It appears that an efficient procedure to follow when the standard HF approach is used is first to examine the effects which model changes have on single particle properties (radii, E2 rates, inelastic nucleon scattering, etc.), and then when one is satisfied that the moder wave functions have improved significantly, to examine properties such as projected spectra which are much more involved in terms of the calculational tools required.

REFERENCES

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3. A. Volkov, Nucl. Phys. 74, 33(1965).

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5. W. F. Ford and R. C. Braley. Proposed NASA Technical Memorandum.

TABLE I. - OSCILLATOR PARAMETER, b = 1.69 fm

Nucleus	Basis	$\langle R^2 \rangle^{1/2}$, fm	B(E2; 0^+ - 2^+), $e^2 \cdot fm^4$	E_{HF}, MeV	Δ, MeV
^{20}Ne	HO	2.65	77.3	-118.43	10.6
	WS	2.84	140.8	-84.98	8.0
^{24}Mg	HO	2.75	111.2	-139.31	0.38
	WS	2.96	174.4	-87.54	0.11
^{28}Si	HO	2.81	157.6	-192.15	11.51
	WS	3.09	274.9	-116.03	8.6
^{32}S	HO	2.86	112.4	-232.83	0.38
	WS	3.17	182.7	-134.15	0.22

TABLE II. - OSCILLATOR PARAMETER, b = 1.924 fm

Nucleus	Basis	$\langle R^2 \rangle^{1/2}$,	B(E2; 0^+ - 2^+), $e^2 \cdot fm^4$	E_{HF}, MeV	Δ, MeV
^{20}Ne	HO	3.01	135.7	-98.37	8.3
	WS	2.84	140.8	-84.98	8.0
^{24}Mg	HO	3.12	191.2	-116.77	0.24
	WS	2.96	174.4	-87.54	0.11
^{28}Si	HO	3.20	269.8	-160.15	9.1
	WS	3.09	274.9	-116.03	8.6
^{32}S	HO	3.25	192.8	-193.75	0.24
	WS	3.17	182.7	-134.15	0.22

TABLE III. - EXPERIMENTAL

E2 RATES AND RADII

	$B(E2;\ 0^+ - 2^+)$, $e^2 \cdot fm^4$	$\langle R^2 \rangle^{1/2}$, fm
^{20}Ne	286±15	2.79±0.03
^{24}Mg	436±46	3.02±0.03
^{28}Si	327±17	3.08±0.06
^{32}S	217±30	3.23±0.07

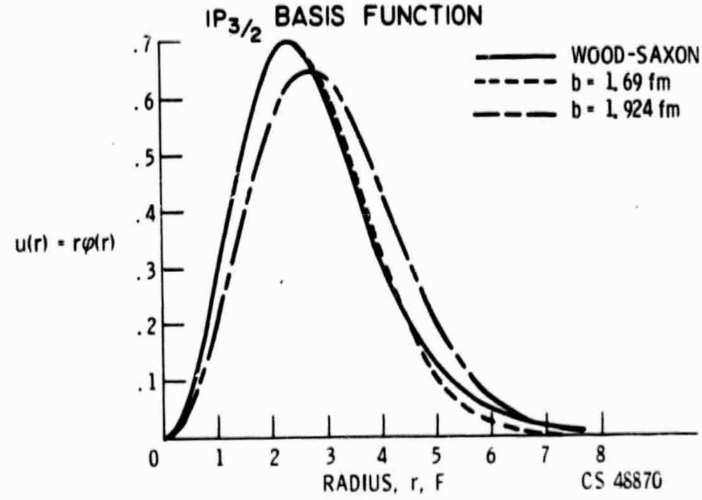

Figure 1

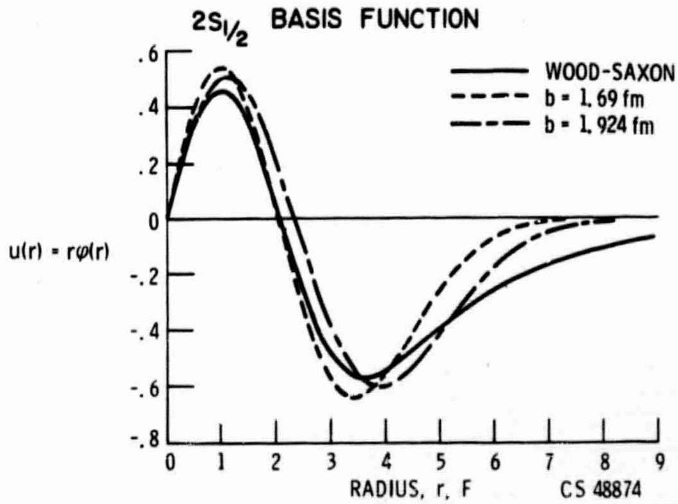

Figure 2

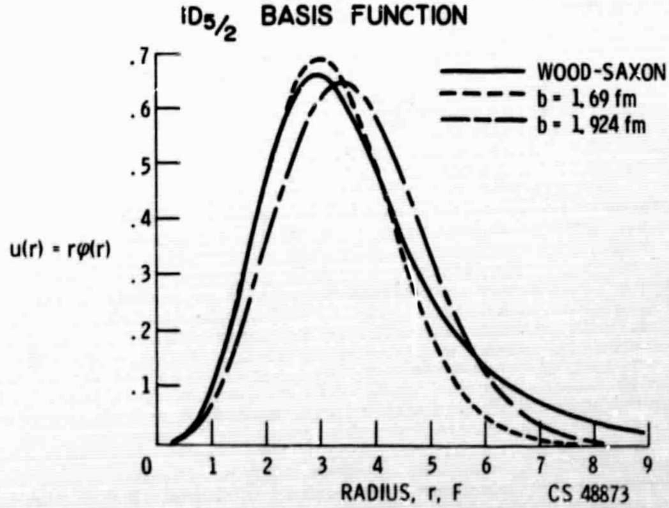

Figure 3

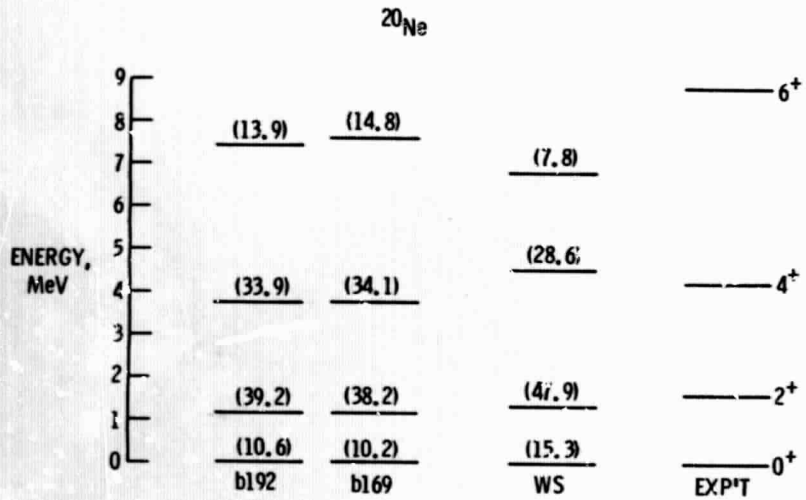

Figure 4. - Projected spectra for ^{20}Ne using bases corresponding to the spaces defined in the text. Exp't refers to experiment.

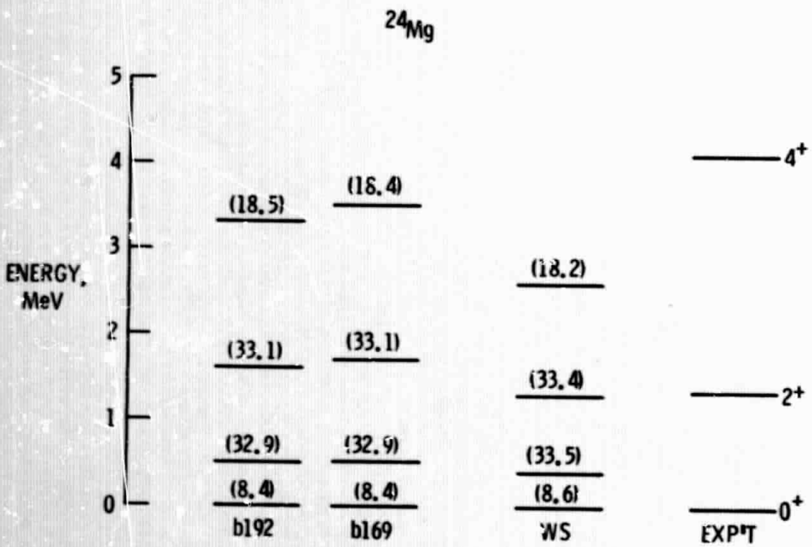

Figure 5. - Projected spectra for ^{24}Mg.

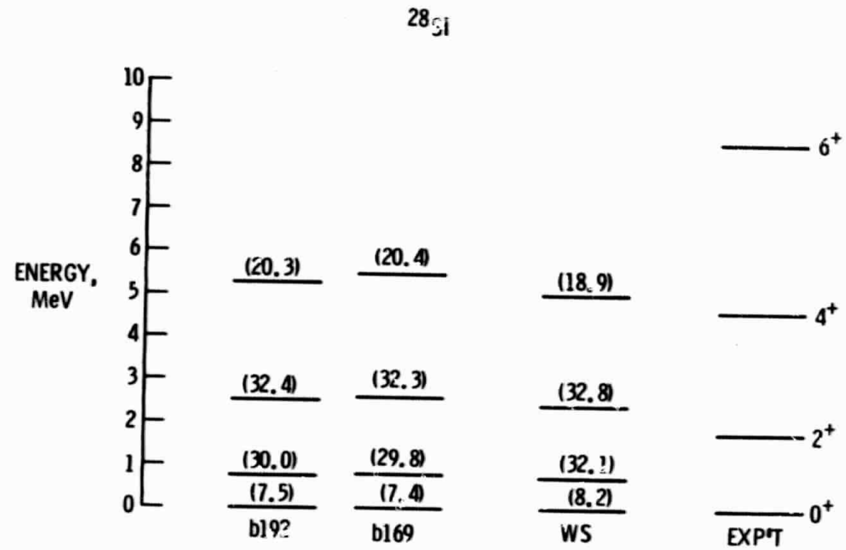

Figure 6. - Projected spectra for ^{28}Si.

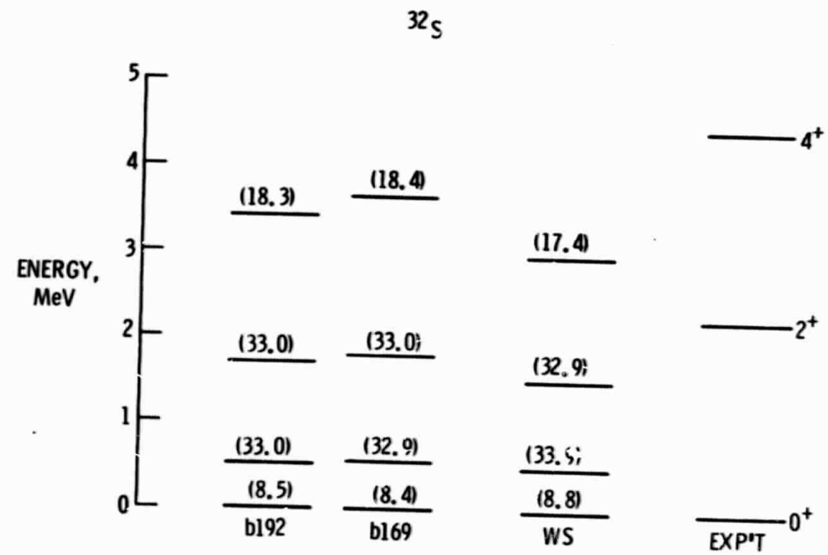

Figure 7. - Projected spectra for ^{32}S.